



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:21 PM UTC

PDB ID : 3VYG / pdb_00003vyg
Title : Crystal structure of Thiocyanate hydrolase mutant R136W
Authors : Yamanaka, Y.; Sato, M.; Arakawa, T.; Namima, S.; Hori, S.; Ohtaki, A.;
Noguchi, K.; Katayama, Y.; Yohda, M.; Odaka, M.
Deposited on : 2012-09-25
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

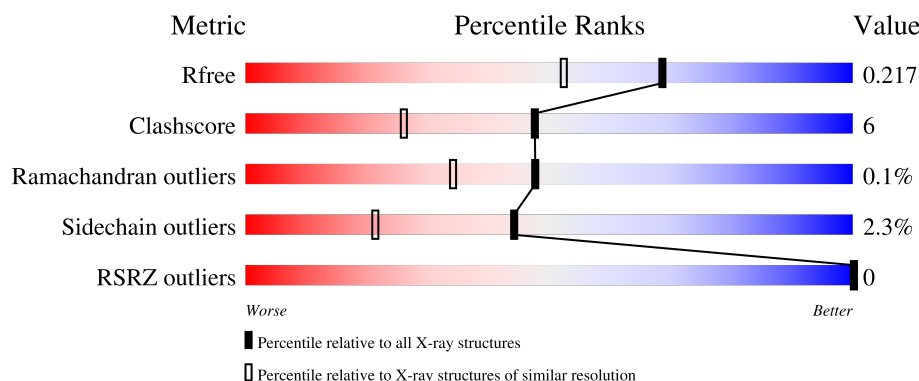
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	126	
1	D	126	
1	G	126	
1	J	126	
2	B	157	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	157	
2	H	157	
2	K	157	
3	C	243	
3	F	243	
3	I	243	
3	L	243	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17343 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thiocyanate hydrolase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	15	0	0
			974	620	162	188	4			
1	D	119	Total	C	N	O	S	10	1	0
			973	620	161	188	4			
1	G	120	Total	C	N	O	S	16	1	0
			982	626	163	189	4			
1	J	120	Total	C	N	O	S	8	1	0
			981	625	163	189	4			

- Molecule 2 is a protein called Thiocyanate hydrolase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	2	0
			1244	787	224	227	6			
2	E	151	Total	C	N	O	S	0	3	0
			1248	790	226	226	6			
2	H	151	Total	C	N	O	S	0	0	0
			1226	775	221	224	6			
2	K	151	Total	C	N	O	S	0	0	0
			1224	773	221	224	6			

- Molecule 3 is a protein called Thiocyanate hydrolase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	10	2	0
			1743	1114	306	315	8			
3	F	217	Total	C	N	O	S	0	2	0
			1744	1113	306	317	8			
3	I	217	Total	C	N	O	S	7	0	0
			1727	1103	302	314	8			
3	L	217	Total	C	N	O	S	17	1	0
			1733	1107	303	315	8			

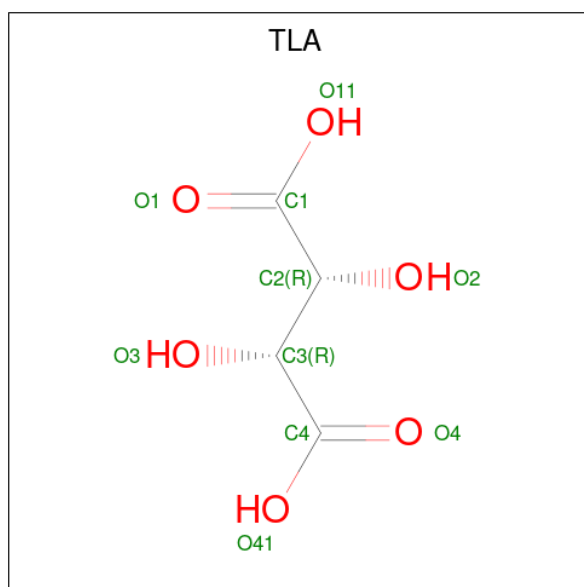
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	136	TRP	ARG	engineered mutation	UNP O66188
F	136	TRP	ARG	engineered mutation	UNP O66188
I	136	TRP	ARG	engineered mutation	UNP O66188
L	136	TRP	ARG	engineered mutation	UNP O66188

- Molecule 4 is COBALT (III) ION (CCD ID: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Co 1 1	0	0
4	F	1	Total Co 1 1	0	0
4	I	1	Total Co 1 1	0	0
4	L	1	Total Co 1 1	0	0

- Molecule 5 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 4 6	0	0
5	F	1	Total C O 10 4 6	0	0
5	I	1	Total C O 10 4 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	129	Total	O	0	0
			129	129		
6	C	214	Total	O	0	0
			214	214		
6	D	78	Total	O	0	0
			78	78		
6	E	128	Total	O	0	0
			128	128		
6	F	189	Total	O	0	0
			189	189		
6	G	84	Total	O	0	0
			84	84		
6	H	107	Total	O	0	0
			107	107		
6	I	148	Total	O	0	0
			148	148		
6	J	90	Total	O	0	0
			90	90		
6	K	109	Total	O	0	0
			109	109		
6	L	153	Total	O	0	0
			153	153		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

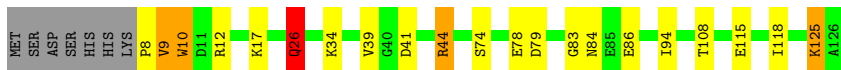
- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain A: 



- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain D: 



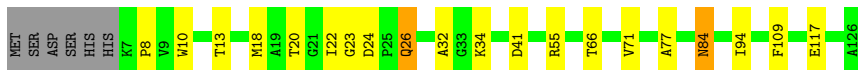
- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain G: 



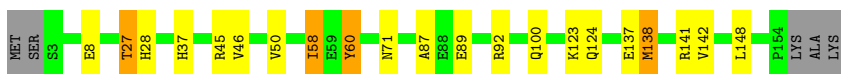
- Molecule 1: Thiocyanate hydrolase subunit alpha

Chain J: 



- Molecule 2: Thiocyanate hydrolase subunit beta

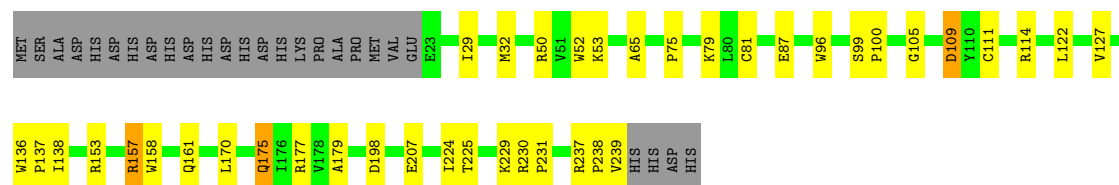
Chain B: 



- Molecule 2: Thiocyanate hydrolase subunit beta

Chain E: 

Chain L: 73% 15% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.45Å 172.40Å 172.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.96 – 1.72 33.96 – 1.72	Depositor EDS
% Data completeness (in resolution range)	96.5 (33.96-1.72) 96.2 (33.96-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.52 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.218 0.188 , 0.217	Depositor DCC
R_{free} test set	17919 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.447 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17343	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3CO, TLA, CSO, CSD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.66	8/1000 (0.8%)	1.33	3/1354 (0.2%)
1	D	1.68	10/999 (1.0%)	1.34	8/1353 (0.6%)
1	G	1.73	7/1008 (0.7%)	1.40	6/1365 (0.4%)
1	J	1.69	13/1007 (1.3%)	1.41	5/1364 (0.4%)
2	B	1.62	7/1279 (0.5%)	1.46	4/1741 (0.2%)
2	E	1.61	5/1283 (0.4%)	1.44	1/1746 (0.1%)
2	H	1.65	11/1258 (0.9%)	1.45	7/1712 (0.4%)
2	K	1.65	12/1256 (1.0%)	1.37	11/1709 (0.6%)
3	C	1.75	15/1776 (0.8%)	1.47	6/2425 (0.2%)
3	F	1.77	18/1777 (1.0%)	1.45	9/2426 (0.4%)
3	I	1.64	14/1757 (0.8%)	1.43	10/2400 (0.4%)
3	L	1.76	20/1766 (1.1%)	1.38	5/2412 (0.2%)
All	All	1.69	140/16166 (0.9%)	1.42	75/22007 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	50	ARG	CD-NE	-15.38	1.24	1.46
2	H	29	ALA	CA-CB	13.93	1.62	1.52
2	K	16	VAL	CA-CB	10.03	1.68	1.54
1	D	9	VAL	CA-CB	9.35	1.66	1.54
3	L	79	LYS	CD-CE	-9.06	1.25	1.52
3	L	127	VAL	CA-CB	8.18	1.66	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ILE	CA-CB	-8.17	1.44	1.54
1	J	32	ALA	CA-CB	7.94	1.67	1.53
1	D	34	LYS	CB-CG	7.85	1.75	1.52
3	L	157	ARG	CA-C	7.78	1.62	1.52
3	I	65	ALA	N-CA	7.77	1.55	1.46
1	D	39	VAL	C-O	7.75	1.31	1.24
3	L	122	LEU	N-CA	7.61	1.55	1.46
1	D	26	GLN	N-CA	7.46	1.55	1.46
3	C	149	PRO	N-CA	-7.28	1.38	1.47
3	L	179	ALA	CA-CB	6.92	1.62	1.53
1	J	66	THR	N-CA	6.90	1.54	1.46
3	L	87	GLU	C-O	6.85	1.31	1.24
3	F	226	VAL	C-O	6.83	1.30	1.23
3	C	92	VAL	CA-CB	6.82	1.62	1.54
3	L	109	ASP	CG-OD2	6.78	1.38	1.25
1	G	39	VAL	C-O	6.74	1.30	1.24
2	K	50	VAL	N-CA	6.72	1.55	1.46
3	F	219	VAL	CA-C	-6.71	1.45	1.52
1	J	24	ASP	C-O	-6.60	1.17	1.25
3	L	87	GLU	N-CA	6.56	1.54	1.46
2	H	50	VAL	N-CA	6.50	1.54	1.46
2	E	120	LEU	N-CA	6.37	1.54	1.46
1	G	24	ASP	CA-C	6.36	1.58	1.52
2	K	29	ALA	CA-CB	6.31	1.63	1.53
3	C	226	VAL	C-O	6.31	1.30	1.24
1	G	35	SER	N-CA	6.26	1.53	1.46
1	G	58	THR	N-CA	6.25	1.54	1.46
3	F	105	GLY	N-CA	6.23	1.52	1.45
1	A	39	VAL	C-O	6.22	1.30	1.24
3	F	62	LEU	N-CA	6.18	1.52	1.46
3	L	138	ILE	CA-CB	-6.15	1.48	1.54
2	B	50	VAL	CA-CB	-6.12	1.48	1.54
3	C	70	LYS	C-O	6.11	1.31	1.24
3	L	137	PRO	N-CA	6.09	1.55	1.47
1	G	125	LYS	CB-CG	-6.06	1.34	1.52
3	I	68	VAL	CA-CB	-6.04	1.47	1.54
3	F	92	VAL	CA-CB	6.04	1.61	1.54
3	I	109	ASP	CG-OD2	6.03	1.36	1.25
3	I	157	ARG	CA-C	6.02	1.60	1.52
3	F	217	VAL	C-O	6.02	1.31	1.24
3	I	87	GLU	C-O	5.88	1.30	1.24
3	L	175	GLN	C-O	5.88	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	23	GLY	N-CA	5.86	1.50	1.45
3	C	189	VAL	CA-CB	5.84	1.61	1.54
2	K	58	ILE	CA-CB	5.84	1.65	1.55
1	A	9	VAL	CA-CB	5.79	1.62	1.54
2	K	92	ARG	CZ-NH1	5.78	1.40	1.32
2	H	29	ALA	C-O	5.77	1.26	1.23
2	B	46	VAL	CA-CB	5.73	1.61	1.54
3	F	60	GLY	N-CA	5.72	1.52	1.44
3	L	161	GLN	CA-C	-5.72	1.45	1.52
1	J	41	ASP	C-O	5.72	1.30	1.23
3	I	127	VAL	CA-CB	5.70	1.63	1.54
3	I	122	LEU	N-CA	5.68	1.52	1.46
2	K	99	GLY	N-CA	5.68	1.51	1.45
3	C	174	VAL	CA-CB	-5.67	1.47	1.54
3	F	174	VAL	CA-CB	-5.67	1.48	1.54
1	J	117	GLU	N-CA	5.66	1.52	1.46
3	C	114	ARG	N-CA	5.59	1.52	1.46
1	A	44	ARG	C-O	-5.55	1.17	1.23
2	K	131	LEU	C-O	5.53	1.30	1.24
2	K	116	ALA	CA-CB	5.53	1.62	1.53
3	C	109	ASP	CG-OD2	5.53	1.35	1.25
1	A	125	LYS	CB-CG	-5.53	1.35	1.52
2	K	17	ALA	CA-CB	-5.51	1.44	1.53
2	H	92	ARG	CZ-NH1	5.49	1.40	1.32
3	F	220	PRO	CA-C	5.47	1.59	1.52
1	G	23	GLY	N-CA	5.46	1.51	1.45
2	B	60	TYR	N-CA	5.46	1.53	1.46
2	K	22	ALA	CA-CB	5.44	1.62	1.53
3	C	192	VAL	N-CA	5.43	1.52	1.46
3	I	137	PRO	N-CA	5.42	1.54	1.47
1	D	17	LYS	CD-CE	-5.41	1.36	1.52
3	F	109	ASP	CG-OD2	5.40	1.35	1.25
3	I	176	ILE	CA-CB	5.39	1.60	1.54
2	H	44	THR	N-CA	5.39	1.53	1.46
3	C	221	LYS	CA-C	-5.37	1.48	1.52
3	L	122	LEU	C-O	5.36	1.30	1.23
2	K	106	MET	C-O	5.35	1.29	1.23
1	D	118	ILE	CA-CB	5.35	1.61	1.54
3	F	127	VAL	CA-CB	5.32	1.63	1.55
2	K	80	ALA	CA-CB	5.31	1.61	1.53
1	A	78	GLU	CA-C	5.31	1.60	1.52
3	C	58	THR	C-O	5.31	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	27	THR	CA-CB	5.30	1.61	1.53
1	J	71	VAL	N-CA	-5.28	1.39	1.46
3	C	62	LEU	N-CA	5.28	1.51	1.46
1	J	77	ALA	CA-CB	5.27	1.61	1.53
1	A	55	ARG	N-CA	5.27	1.52	1.46
2	H	116	ALA	CA-CB	5.24	1.61	1.53
3	I	197	THR	CA-CB	5.24	1.61	1.53
2	B	123	LYS	CA-C	5.24	1.60	1.52
2	H	128	LEU	CA-CB	5.22	1.61	1.53
3	L	65	ALA	N-CA	5.22	1.52	1.46
1	J	13	THR	CA-C	-5.22	1.45	1.52
3	F	73	LEU	N-CA	5.22	1.52	1.46
1	D	44	ARG	C-O	-5.21	1.17	1.23
3	F	117	ALA	N-CA	5.21	1.52	1.46
3	F	149	PRO	N-CA	-5.21	1.40	1.47
2	H	80	ALA	CA-CB	5.20	1.61	1.53
1	G	24	ASP	C-O	-5.20	1.18	1.25
2	E	60	TYR	N-CA	5.20	1.52	1.46
2	E	80	ALA	CA-CB	5.20	1.61	1.53
3	C	125	VAL	N-CA	5.19	1.52	1.46
1	J	55	ARG	CZ-NH1	5.19	1.40	1.32
1	D	78	GLU	CA-C	5.18	1.59	1.52
1	J	20	THR	N-CA	5.17	1.52	1.46
3	F	186	ARG	CD-NE	5.17	1.53	1.46
3	C	113	LEU	N-CA	5.16	1.52	1.46
3	L	81	CYS	N-CA	5.16	1.52	1.46
2	B	87	ALA	CA-CB	5.16	1.61	1.53
2	B	50	VAL	N-CA	5.15	1.51	1.46
3	I	118	ASP	N-CA	5.14	1.52	1.45
3	L	138	ILE	CA-C	5.14	1.59	1.52
3	L	114	ARG	CZ-NH1	5.11	1.40	1.32
3	L	136	TRP	N-CA	5.10	1.51	1.46
3	L	52	TRP	CA-CB	5.09	1.61	1.53
1	A	52	PHE	N-CA	5.09	1.52	1.46
3	I	179	ALA	CA-CB	5.07	1.60	1.53
1	J	22	ILE	CA-C	5.07	1.59	1.52
2	E	72	THR	N-CA	5.06	1.52	1.46
2	E	87	ALA	CA-CB	5.06	1.61	1.53
2	H	70	LEU	CG-CD1	5.05	1.69	1.52
1	D	41	ASP	C-O	5.04	1.29	1.23
2	B	89	GLU	CA-C	5.04	1.59	1.52
3	I	64	ALA	CA-CB	5.04	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	61	PRO	N-CA	-5.04	1.41	1.47
2	H	5	ILE	N-CA	5.04	1.52	1.46
3	F	143	PRO	C-O	5.03	1.29	1.23
3	C	78	LYS	CA-CB	5.03	1.61	1.53
3	I	89	SER	CA-C	5.03	1.59	1.52
1	J	24	ASP	CA-C	5.03	1.56	1.52
3	F	230	ARG	CA-C	5.02	1.57	1.52
1	D	10	TRP	CA-C	-5.02	1.46	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	23	GLU	CB-CG-CD	-10.46	94.81	112.60
3	L	79	LYS	CG-CD-CE	10.18	134.70	111.30
2	B	138	MET	CG-SD-CE	-9.79	79.36	100.90
3	I	238	PRO	N-CA-C	8.78	124.58	111.41
3	L	238	PRO	N-CA-C	8.10	125.20	111.68
3	L	50	ARG	CG-CD-NE	8.04	129.69	112.00
2	E	138	MET	CG-SD-CE	-7.99	83.32	100.90
3	F	119	SER	CA-C-N	-7.85	112.13	119.82
3	F	119	SER	C-N-CA	-7.85	112.13	119.82
3	L	237	ARG	CA-C-N	7.79	128.40	120.14
3	L	237	ARG	C-N-CA	7.79	128.40	120.14
3	I	237	ARG	CA-C-N	7.16	127.11	120.03
3	I	237	ARG	C-N-CA	7.16	127.11	120.03
1	A	34	LYS	CA-CB-CG	-7.04	100.01	114.10
3	I	88	ALA	N-CA-C	7.04	118.96	111.28
2	K	128	LEU	N-CA-C	-7.03	103.66	111.82
1	D	17	LYS	CG-CD-CE	6.88	127.12	111.30
2	H	46	VAL	CA-C-N	-6.63	112.88	120.04
2	H	46	VAL	C-N-CA	-6.63	112.88	120.04
1	D	125	LYS	CA-CB-CG	6.39	126.89	114.10
1	G	109	PHE	CA-C-N	6.33	128.77	120.28
1	G	109	PHE	C-N-CA	6.33	128.77	120.28
3	I	102	THR	N-CA-C	6.32	118.97	111.71
3	F	190	MET	CA-C-N	-6.28	114.18	120.21
3	F	190	MET	C-N-CA	-6.28	114.18	120.21
3	I	136	TRP	O-C-N	6.17	126.51	120.71
1	J	109	PHE	CA-C-N	6.15	129.13	120.28
1	J	109	PHE	C-N-CA	6.15	129.13	120.28
1	J	84	ASN	CA-C-N	-6.07	112.96	122.49
1	J	84	ASN	C-N-CA	-6.07	112.96	122.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	46	VAL	CA-C-N	-5.96	113.67	119.87
2	K	46	VAL	C-N-CA	-5.96	113.67	119.87
2	H	26	GLN	CA-C-N	-5.92	114.83	123.00
2	H	26	GLN	C-N-CA	-5.92	114.83	123.00
1	D	9	VAL	N-CA-CB	5.85	119.48	111.41
2	K	45	ARG	CB-CG-CD	5.79	124.63	111.30
1	G	68	VAL	N-CA-C	-5.79	107.62	113.47
3	F	208	ILE	CA-C-N	-5.78	116.24	122.59
3	F	208	ILE	C-N-CA	-5.78	116.24	122.59
1	D	74	SER	N-CA-CB	-5.76	105.86	111.27
1	D	118	ILE	CA-C-N	-5.71	114.72	120.31
1	D	118	ILE	C-N-CA	-5.71	114.72	120.31
2	B	50	VAL	N-CA-C	-5.67	107.60	113.10
1	D	12	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	B	27	THR	OG1-CB-CG2	-5.64	98.01	109.30
3	F	193	ARG	CA-C-N	-5.63	114.77	120.85
3	F	193	ARG	C-N-CA	-5.63	114.77	120.85
1	G	94	ILE	CB-CA-C	-5.58	102.36	110.63
2	K	118	ARG	CG-CD-NE	-5.52	99.86	112.00
3	C	80	LEU	N-CA-C	-5.50	105.20	111.14
3	I	100	PRO	CB-CA-C	-5.47	104.25	110.92
3	C	119	SER	CA-C-N	-5.44	114.21	119.87
3	C	119	SER	C-N-CA	-5.44	114.21	119.87
1	G	84	ASN	CA-C-N	-5.42	113.97	122.49
1	G	84	ASN	C-N-CA	-5.42	113.97	122.49
3	I	77	TYR	N-CA-C	-5.34	105.53	111.36
2	B	46	VAL	CG1-CB-CG2	-5.28	99.18	110.80
2	H	152	LEU	CA-C-N	-5.27	114.95	120.38
2	H	152	LEU	C-N-CA	-5.27	114.95	120.38
2	K	152	LEU	CA-C-N	-5.27	114.95	120.38
2	K	152	LEU	C-N-CA	-5.27	114.95	120.38
3	I	186	ARG	N-CA-C	-5.21	101.38	109.72
1	J	94	ILE	CB-CA-C	-5.20	102.94	110.63
2	K	39	LEU	N-CA-C	5.17	116.91	111.28
2	K	26	GLN	CA-C-N	-5.13	115.92	123.00
2	K	26	GLN	C-N-CA	-5.13	115.92	123.00
2	K	112	TRP	N-CA-C	-5.10	105.72	111.28
1	A	118	ILE	CA-C-N	-5.09	115.32	120.31
1	A	118	ILE	C-N-CA	-5.09	115.32	120.31
3	I	173	GLU	N-CA-C	-5.08	106.93	113.23
3	C	118	ASP	N-CA-C	-5.07	103.84	110.53
2	H	45	ARG	CB-CG-CD	5.06	122.94	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	ARG	NE-CZ-NH1	-5.06	116.44	121.50
3	C	189	VAL	N-CA-CB	-5.02	104.97	110.99
3	F	195	GLU	CA-CB-CG	-5.01	104.09	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	4	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	974	0	926	17	0
1	D	973	0	924	17	0
1	G	982	0	936	14	0
1	J	981	0	934	10	0
2	B	1244	0	1211	24	0
2	E	1248	0	1222	29	0
2	H	1226	0	1193	19	0
2	K	1224	0	1186	24	0
3	C	1743	0	1755	17	0
3	F	1744	0	1750	13	0
3	I	1727	0	1732	31	0
3	L	1733	0	1740	16	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	C	10	0	4	0	0
5	F	10	0	4	0	0
5	I	10	0	4	0	0
5	L	10	0	4	0	0
6	A	71	0	0	1	0
6	B	129	0	0	0	0
6	C	214	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	78	0	0	0	0
6	E	128	0	0	2	0
6	F	189	0	0	0	0
6	G	84	0	0	1	0
6	H	107	0	0	3	0
6	I	148	0	0	4	0
6	J	90	0	0	0	0
6	K	109	0	0	5	0
6	L	153	0	0	2	0
All	All	17343	0	15525	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:47:GLU:HG2	3:I:50:ARG:NH2	1.40	1.32
2:K:65:GLU:OE1	2:K:70:LEU:HB2	1.17	1.27
2:B:137:GLU:OE1	2:B:141:ARG:HD2	1.35	1.22
2:B:137:GLU:OE1	2:B:141:ARG:CD	1.97	1.11
1:D:10:TRP:HZ3	6:H:283:HOH:O	1.36	1.08
2:E:137:GLU:OE1	2:E:141[A]:ARG:HD2	1.53	1.07
3:I:66:ARG:HH11	3:I:66:ARG:HG3	1.04	1.07
1:A:10:TRP:HZ3	6:K:297:HOH:O	1.44	0.98
2:K:65:GLU:OE1	2:K:70:LEU:CB	2.12	0.97
2:K:45:ARG:HD3	6:K:307:HOH:O	1.65	0.97
2:E:58:ILE:HD11	2:E:60:TYR:CE1	2.02	0.95
3:I:66:ARG:HG3	3:I:66:ARG:NH1	1.73	0.94
2:H:134:LYS:HD2	2:H:138:MET:HE2	1.49	0.93
2:E:137:GLU:OE1	2:E:141[A]:ARG:CD	2.17	0.92
3:I:66:ARG:HH11	3:I:66:ARG:CG	1.83	0.92
1:G:26:GLN:H	1:G:26:GLN:HE21	1.18	0.90
1:A:26:GLN:HE21	1:A:26:GLN:H	1.19	0.90
3:I:47:GLU:CG	3:I:50:ARG:HH21	1.87	0.88
2:K:4:SER:N	6:K:274:HOH:O	2.09	0.86
3:I:47:GLU:HG2	3:I:50:ARG:HH21	1.07	0.86
1:D:26:GLN:HE21	1:D:26:GLN:H	1.24	0.85
2:H:45:ARG:HD3	6:H:306:HOH:O	1.77	0.85
1:J:26:GLN:HE21	1:J:26:GLN:H	1.24	0.84
3:I:47:GLU:CG	3:I:50:ARG:NH2	2.35	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:GLN:HE22	3:I:111:CYS:HB2	1.44	0.81
1:J:26:GLN:HE22	3:L:111:CYS:HB2	1.46	0.79
2:E:58:ILE:HD12	2:E:58:ILE:O	1.83	0.78
1:A:26:GLN:HE22	3:C:111:CYS:HB2	1.47	0.78
1:A:38:ASN:ND2	6:A:269:HOH:O	2.17	0.77
3:I:66:ARG:NH1	3:I:66:ARG:CG	2.42	0.75
1:D:26:GLN:HE22	3:F:111:CYS:HB2	1.49	0.75
3:L:175:GLN:HE22	3:L:177:ARG:HH11	1.33	0.74
3:I:175:GLN:HE22	3:I:177:ARG:HH11	1.34	0.74
3:C:153:ARG:HH12	2:K:28:HIS:CD2	2.07	0.73
2:E:28:HIS:CD2	3:I:153:ARG:HH12	2.06	0.73
2:K:45:ARG:HH11	2:K:100:GLN:HE22	1.37	0.72
1:A:7:LYS:NZ	1:J:84:ASN:HD22	1.88	0.72
2:B:58:ILE:HD11	2:B:60:TYR:CE1	2.29	0.68
3:F:153:ARG:HH12	2:H:28:HIS:CD2	2.11	0.68
2:H:45:ARG:HH11	2:H:100:GLN:HE22	1.42	0.67
2:B:28:HIS:CD2	3:L:153:ARG:HH12	2.12	0.67
2:K:58:ILE:HD11	2:K:60:TYR:CE1	2.31	0.66
3:C:175:GLN:HE22	3:C:177:ARG:HH11	1.44	0.65
2:B:138:MET:SD	2:B:148:LEU:HD11	2.37	0.65
2:B:45:ARG:HH11	2:B:100:GLN:HE22	1.45	0.65
2:B:137:GLU:OE1	2:B:141:ARG:HD3	1.96	0.64
3:F:175:GLN:HE22	3:F:177:ARG:HH11	1.45	0.63
1:A:7:LYS:HZ3	1:J:84:ASN:HD22	1.46	0.63
3:C:153:ARG:HH12	2:K:28:HIS:HD2	1.48	0.62
2:E:28:HIS:HD2	3:I:153:ARG:HH12	1.46	0.62
2:B:37:HIS:HE1	2:H:8:GLU:OE1	1.82	0.62
2:H:71:ASN:HD21	3:I:53:LYS:NZ	1.98	0.61
3:F:153:ARG:HH12	2:H:28:HIS:HD2	1.47	0.61
1:A:10:TRP:CZ3	6:K:297:HOH:O	2.32	0.61
2:K:58:ILE:HD11	2:K:60:TYR:CZ	2.36	0.61
2:B:58:ILE:HD13	2:B:58:ILE:O	2.01	0.60
1:A:7:LYS:HD2	2:B:124:GLN:NE2	2.17	0.60
1:D:83:GLY:O	1:G:7:LYS:HE2	2.03	0.59
2:E:8:GLU:OE2	2:K:37:HIS:HE1	1.86	0.59
2:E:11:ARG:HD3	6:K:279:HOH:O	2.03	0.59
1:G:26:GLN:H	1:G:26:GLN:NE2	1.94	0.59
2:B:71:ASN:HD21	3:C:53:LYS:NZ	2.00	0.59
1:D:86:GLU:OE2	1:G:7:LYS:NZ	2.34	0.59
2:K:71:ASN:HD21	3:L:53:LYS:NZ	2.01	0.58
3:I:76:GLU:HG3	6:I:547:HOH:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:VAL:HG21	3:C:24:VAL:HG21	1.84	0.58
2:K:45:ARG:NH1	2:K:100:GLN:HE22	2.02	0.58
3:C:66[A]:ARG:HD3	6:C:583:HOH:O	2.04	0.57
2:B:45:ARG:NH1	2:B:100:GLN:HE22	2.03	0.57
2:E:142:VAL:HG21	3:F:24:VAL:HG21	1.86	0.57
2:K:45:ARG:HH11	2:K:100:GLN:NE2	2.03	0.56
3:I:230:ARG:HB2	3:I:231:PRO:HD2	1.87	0.56
2:B:8:GLU:OE2	2:H:37:HIS:HE1	1.88	0.56
3:C:29[A]:ILE:HD11	6:C:555:HOH:O	2.05	0.56
2:H:45:ARG:O	2:H:45:ARG:HG3	2.05	0.55
2:H:65:GLU:OE1	2:H:70:LEU:HB2	2.06	0.55
3:F:47[B]:GLU:HB2	3:F:50:ARG:NH2	2.21	0.55
2:E:71:ASN:HD21	3:F:53:LYS:NZ	2.05	0.55
3:I:47:GLU:HG2	3:I:50:ARG:HH22	1.58	0.55
1:D:86:GLU:OE2	1:G:7:LYS:HE3	2.07	0.54
2:E:138:MET:SD	2:E:148:LEU:HD11	2.47	0.54
3:L:75:PRO:HD3	6:L:552:HOH:O	2.08	0.53
2:K:58:ILE:HD13	2:K:58:ILE:O	2.06	0.53
1:D:8:PRO:HG3	1:G:10:TRP:CZ3	2.43	0.53
2:H:45:ARG:NH1	2:H:100:GLN:HE22	2.07	0.53
2:K:58:ILE:N	2:K:58:ILE:CD1	2.71	0.53
1:A:7:LYS:HD2	2:B:124:GLN:HE22	1.73	0.53
1:D:26:GLN:HE21	1:D:26:GLN:N	2.01	0.52
2:E:37:HIS:HE1	2:K:8:GLU:OE2	1.91	0.52
2:E:45:ARG:HH11	2:E:100:GLN:HE22	1.57	0.52
1:A:26:GLN:HE21	1:A:26:GLN:N	1.97	0.52
2:E:58:ILE:CD1	2:E:60:TYR:CE1	2.84	0.52
2:E:46:VAL:HG23	2:E:46:VAL:O	2.10	0.51
1:J:26:GLN:H	1:J:26:GLN:NE2	2.03	0.51
1:D:26:GLN:H	1:D:26:GLN:NE2	2.03	0.51
1:G:12:ARG:HD3	6:G:249:HOH:O	2.10	0.51
2:H:148:LEU:HG	3:I:32:MET:HG3	1.93	0.51
1:A:8:PRO:HG3	1:J:10:TRP:CZ3	2.44	0.51
3:L:230:ARG:HB2	3:L:231:PRO:HD2	1.92	0.51
6:E:251:HOH:O	2:K:12:HIS:HE1	1.92	0.51
2:B:28:HIS:HD2	3:L:153:ARG:HH12	1.54	0.50
3:C:119:SER:HB2	3:C:120:PRO:CD	2.41	0.50
3:I:99:SER:N	3:I:100:PRO:CD	2.74	0.50
2:H:138:MET:HE3	3:I:33:ALA:HA	1.93	0.50
2:K:71:ASN:HD21	3:L:53:LYS:HZ2	1.60	0.50
2:H:138:MET:HE1	3:I:36:GLU:CD	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLU:OE2	1:G:7:LYS:CE	2.60	0.50
3:F:26:ASP:OD2	2:H:37:HIS:HD2	1.94	0.49
2:H:45:ARG:HH11	2:H:100:GLN:NE2	2.07	0.49
2:E:58:ILE:HD12	2:E:58:ILE:C	2.38	0.49
1:D:10:TRP:CZ3	6:H:283:HOH:O	2.27	0.48
3:C:42:GLY:HA2	6:C:578:HOH:O	2.13	0.48
1:D:10:TRP:CZ3	2:E:123:LYS:HE2	2.49	0.48
2:E:152:LEU:HD12	2:E:153:PRO:HD2	1.96	0.48
2:B:148:LEU:HG	3:C:32:MET:HE2	1.95	0.48
1:D:108:THR:HG22	3:F:172:SER:HB2	1.96	0.48
2:E:137:GLU:OE1	2:E:141[A]:ARG:CG	2.62	0.48
2:K:53:GLU:HB2	3:L:153:ARG:HG2	1.96	0.48
2:B:71:ASN:HD21	3:C:53:LYS:HZ2	1.61	0.47
3:I:100:PRO:HG3	6:I:494:HOH:O	2.15	0.47
3:L:99:SER:N	3:L:100:PRO:CD	2.77	0.47
2:B:45:ARG:HH11	2:B:100:GLN:NE2	2.12	0.47
2:E:37:HIS:HD2	3:I:26:ASP:OD2	1.98	0.47
2:H:67:ILE:HD12	3:I:237:ARG:HG2	1.97	0.47
3:C:157:ARG:HD3	3:C:158:TRP:CH2	2.50	0.47
3:I:96:TRP:O	3:I:105:GLY:HA2	2.15	0.47
1:A:7:LYS:HZ2	1:J:84:ASN:ND2	2.13	0.46
2:B:58:ILE:CD1	2:B:58:ILE:N	2.78	0.46
3:F:23:GLU:HG3	3:F:24:VAL:N	2.30	0.46
3:I:76:GLU:CG	6:I:547:HOH:O	2.61	0.46
2:K:45:ARG:O	2:K:45:ARG:HG3	2.09	0.46
3:L:100:PRO:HG3	6:L:453:HOH:O	2.14	0.46
1:A:10:TRP:CZ3	1:J:8:PRO:HG3	2.50	0.46
2:B:58:ILE:CD1	2:B:58:ILE:H	2.28	0.46
3:C:26:ASP:OD2	2:K:37:HIS:HD2	1.99	0.45
3:C:67:LEU:C	3:C:67:LEU:HD23	2.42	0.45
2:E:58:ILE:CD1	2:E:58:ILE:C	2.89	0.45
1:G:26:GLN:HE21	1:G:26:GLN:N	2.00	0.45
3:I:157:ARG:HD3	3:I:158:TRP:CH2	2.52	0.45
2:E:58:ILE:CD1	2:E:60:TYR:CD1	3.00	0.45
2:E:45:ARG:O	2:E:45:ARG:HG3	2.15	0.44
2:E:34:GLU:HG3	6:E:324:HOH:O	2.16	0.44
3:I:76:GLU:CB	6:I:547:HOH:O	2.64	0.44
1:D:10:TRP:CZ3	1:G:8:PRO:HG3	2.53	0.44
2:E:148:LEU:HG	3:F:32:MET:HE2	2.00	0.44
2:B:27:THR:HG23	2:E:22:ALA:HA	1.99	0.44
2:K:148:LEU:HG	3:L:32:MET:HG3	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:175:GLN:NE2	3:L:177:ARG:HH11	2.09	0.43
1:A:99:LYS:HG2	1:A:100:ASP:N	2.32	0.43
3:L:157:ARG:HD3	3:L:158:TRP:CH2	2.54	0.43
2:H:71:ASN:HD21	3:I:53:LYS:HZ2	1.65	0.43
2:B:92:ARG:HD2	2:B:92:ARG:C	2.43	0.43
2:E:58:ILE:O	2:E:58:ILE:CD1	2.61	0.43
3:L:207:GLU:HG2	3:L:225:THR:CG2	2.49	0.43
2:K:58:ILE:N	2:K:58:ILE:HD12	2.34	0.42
1:A:26:GLN:H	1:A:26:GLN:NE2	2.01	0.42
1:D:79:ASP:HB3	1:D:84:ASN:O	2.18	0.42
2:B:58:ILE:HD13	2:B:58:ILE:H	1.85	0.42
3:L:96:TRP:O	3:L:105:GLY:HA2	2.19	0.42
3:F:157:ARG:HD3	3:F:158:TRP:CH2	2.54	0.42
1:A:79:ASP:HB3	1:A:84:ASN:O	2.20	0.42
3:C:127:VAL:HG22	3:C:128:CYS:N	2.35	0.42
2:E:148:LEU:CD1	3:F:32:MET:HE2	2.49	0.42
3:C:35:ARG:HH11	3:C:35:ARG:HD2	1.64	0.42
2:K:58:ILE:CD1	2:K:58:ILE:H	2.32	0.42
3:I:136:TRP:CH2	3:I:141:GLN:HB2	2.54	0.41
1:A:8:PRO:HG3	1:J:10:TRP:CH2	2.56	0.41
1:J:26:GLN:HE21	1:J:26:GLN:N	2.04	0.41
1:D:10:TRP:CE3	1:G:8:PRO:HG3	2.56	0.41
2:H:53:GLU:HB2	3:I:153:ARG:HG2	2.01	0.41
2:E:128:LEU:HD12	2:E:128:LEU:HA	1.85	0.41
1:D:94[A]:ILE:O	1:D:115:GLU:HA	2.21	0.40
1:G:111:ASN:O	3:I:175:GLN:HG3	2.21	0.40
1:G:58:THR:HA	1:G:61:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
1	D	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
1	G	119/126 (94%)	114 (96%)	5 (4%)	0	100	100
1	J	119/126 (94%)	115 (97%)	4 (3%)	0	100	100
2	B	152/157 (97%)	147 (97%)	5 (3%)	0	100	100
2	E	152/157 (97%)	148 (97%)	4 (3%)	0	100	100
2	H	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
2	K	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
3	C	215/243 (88%)	206 (96%)	8 (4%)	1 (0%)	24	11
3	F	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
3	I	213/243 (88%)	207 (97%)	6 (3%)	0	100	100
3	L	214/243 (88%)	209 (98%)	5 (2%)	0	100	100
All	All	1933/2104 (92%)	1874 (97%)	58 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	132	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/108 (94%)	97 (95%)	5 (5%)	22	4
1	D	102/108 (94%)	98 (96%)	4 (4%)	28	7
1	G	103/108 (95%)	101 (98%)	2 (2%)	50	27
1	J	103/108 (95%)	100 (97%)	3 (3%)	37	14
2	B	131/134 (98%)	130 (99%)	1 (1%)	73	61
2	E	132/134 (98%)	131 (99%)	1 (1%)	73	61
2	H	129/134 (96%)	127 (98%)	2 (2%)	55	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	128/134 (96%)	126 (98%)	2 (2%)	55	34
3	C	190/212 (90%)	189 (100%)	1 (0%)	81	71
3	F	190/212 (90%)	189 (100%)	1 (0%)	81	71
3	I	188/212 (89%)	179 (95%)	9 (5%)	23	4
3	L	189/212 (89%)	182 (96%)	7 (4%)	30	8
All	All	1687/1816 (93%)	1649 (98%)	38 (2%)	44	21

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	17	LYS
1	A	18	MET
1	A	26	GLN
1	A	99	LYS
2	B	58	ILE
3	C	141	GLN
1	D	9	VAL
1	D	26	GLN
1	D	44	ARG
1	D	125	LYS
2	E	58	ILE
3	F	141	GLN
1	G	18	MET
1	G	26	GLN
2	H	46	VAL
2	H	150	GLU
3	I	47	GLU
3	I	50	ARG
3	I	66	ARG
3	I	107	PRO
3	I	170	LEU
3	I	198	ASP
3	I	224	ILE
3	I	229	LYS
3	I	239	VAL
1	J	18	MET
1	J	26	GLN
1	J	34	LYS
2	K	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	58	ILE
3	L	29	ILE
3	L	109	ASP
3	L	170	LEU
3	L	198	ASP
3	L	224	ILE
3	L	229	LYS
3	L	239	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	111	ASN
2	B	28	HIS
2	B	37	HIS
2	B	71	ASN
2	B	100	GLN
2	B	124	GLN
3	C	141	GLN
3	C	175	GLN
1	D	26	GLN
1	D	84	ASN
1	D	111	ASN
2	E	28	HIS
2	E	37	HIS
2	E	71	ASN
2	E	100	GLN
2	E	124	GLN
3	F	103	GLN
3	F	169	GLN
3	F	175	GLN
1	G	26	GLN
2	H	26	GLN
2	H	28	HIS
2	H	37	HIS
2	H	71	ASN
2	H	100	GLN
3	I	169	GLN
3	I	175	GLN
1	J	26	GLN
1	J	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	111	ASN
2	K	12	HIS
2	K	26	GLN
2	K	28	HIS
2	K	37	HIS
2	K	71	ASN
2	K	100	GLN
2	K	124	GLN
3	L	175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	CSD	F	131	4,3	4,7,8	1.06	0	1,8,10	0.86	0
3	CSD	L	131	4,3	4,7,8	0.76	0	1,8,10	1.62	0
3	CSO	C	133	4,3	3,6,7	1.14	0	1,6,8	0.07	0
3	CSO	F	133	4,3	3,6,7	1.06	0	1,6,8	0.01	0
3	CSO	L	133	4,3	3,6,7	1.13	0	1,6,8	0.26	0
3	CSO	I	133	4,3	3,6,7	1.45	0	1,6,8	0.27	0
3	CSD	I	131	4,3	4,7,8	1.21	1 (25%)	1,8,10	1.57	0
3	CSD	C	131	4,3	4,7,8	2.03	1 (25%)	1,8,10	2.55	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CSD	F	131	4,3	-	0/2/6/8	-
3	CSD	L	131	4,3	-	0/2/6/8	-
3	CSO	C	133	4,3	-	0/1/5/7	-
3	CSO	F	133	4,3	-	0/1/5/7	-
3	CSO	L	133	4,3	-	0/1/5/7	-
3	CSO	I	133	4,3	-	0/1/5/7	-
3	CSD	I	131	4,3	-	0/2/6/8	-
3	CSD	C	131	4,3	-	0/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	131	CSD	OD1-SG	-3.66	1.44	1.47
3	I	131	CSD	OD1-SG	-2.38	1.45	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	131	CSD	OD1-SG-CB	-2.55	100.91	105.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TLA	F	302	-	9,9,9	1.19	0	12,12,12	1.32	2 (16%)
5	TLA	L	302	-	9,9,9	1.22	1 (11%)	12,12,12	0.87	0
5	TLA	I	302	-	9,9,9	1.17	0	12,12,12	0.88	0
5	TLA	C	302	-	9,9,9	1.41	2 (22%)	12,12,12	1.61	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TLA	F	302	-	-	0/12/12/12	-
5	TLA	L	302	-	-	0/12/12/12	-
5	TLA	I	302	-	-	0/12/12/12	-
5	TLA	C	302	-	-	0/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	TLA	O41-C4	-2.58	1.22	1.30
5	C	302	TLA	O1-C1	2.35	1.29	1.22
5	C	302	TLA	C2-C1	2.12	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	302	TLA	O11-C1-O1	3.57	132.19	124.08
5	F	302	TLA	O41-C4-C3	2.29	119.67	113.31
5	F	302	TLA	O11-C1-O1	2.24	129.17	124.08
5	C	302	TLA	O41-C4-C3	2.23	119.52	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	120/126 (95%)	-0.95	0 100 100	13, 20, 30, 38	4 (3%)
1	D	119/126 (94%)	-0.96	0 100 100	8, 20, 30, 37	4 (3%)
1	G	120/126 (95%)	-1.04	0 100 100	8, 16, 29, 43	6 (5%)
1	J	120/126 (95%)	-1.08	0 100 100	11, 16, 28, 33	3 (2%)
2	B	152/157 (96%)	-1.05	0 100 100	7, 16, 30, 39	2 (1%)
2	E	151/157 (96%)	-1.01	0 100 100	7, 16, 31, 37	3 (1%)
2	H	151/157 (96%)	-0.90	0 100 100	12, 19, 39, 48	0
2	K	151/157 (96%)	-0.89	0 100 100	12, 18, 39, 50	0
3	C	215/243 (88%)	-1.01	0 100 100	7, 17, 27, 37	6 (2%)
3	F	215/243 (88%)	-1.00	0 100 100	11, 17, 28, 45	2 (0%)
3	I	215/243 (88%)	-0.94	0 100 100	12, 19, 35, 49	2 (0%)
3	L	215/243 (88%)	-0.91	0 100 100	12, 19, 35, 53	6 (2%)
All	All	1944/2104 (92%)	-0.98	0 100 100	7, 18, 33, 53	38 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CSD	C	131	8/9	0.99	0.04	12,15,18,18	2
3	CSO	C	133	7/8	0.99	0.05	13,14,20,29	1
3	CSO	F	133	7/8	0.99	0.05	13,15,20,31	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CSO	I	133	7/8	0.99	0.04	12,14,21,32	1
3	CSD	L	131	8/9	0.99	0.04	12,15,17,17	2
3	CSO	L	133	7/8	0.99	0.04	13,14,21,33	1
3	CSD	I	131	8/9	1.00	0.04	12,16,17,18	2
3	CSD	F	131	8/9	1.00	0.03	12,15,18,19	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TLA	C	302	10/10	0.99	0.05	18,27,34,37	0
5	TLA	F	302	10/10	0.99	0.04	20,24,34,35	0
5	TLA	I	302	10/10	0.99	0.04	18,21,30,32	0
5	TLA	L	302	10/10	0.99	0.04	20,22,28,32	0
4	3CO	C	301	1/1	1.00	0.01	12,12,12,12	1
4	3CO	F	301	1/1	1.00	0.02	12,12,12,12	1
4	3CO	I	301	1/1	1.00	0.01	13,13,13,13	1
4	3CO	L	301	1/1	1.00	0.01	13,13,13,13	1

6.5 Other polymers [i](#)

There are no such residues in this entry.